

Benzoyl-phosphonic acid dimethyl ester

Inchi: InChI=1S/C9H11O4P/c1-12-14(11,13-2)9(10)8-6-4-3-5-7-8/h3-7H,1-2H3
InchiKey: TWNVJLOWMINFMB-UHFFFAOYSA-N
Formula: C9H11O4P
SMILES: COP(=O)(OC)C(=O)c1ccccc1
Mol. weight [g/mol]: 214.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	2.313		Crippen Method
mcvol	153.550	ml/mol	McGowan Method
rinpol	1572.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1572.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R205206&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/21-982-8/Benzoyl-phosphonic-acid-dimethyl-ester.pdf>

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